



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:19 AM GMT

PDB ID : 1JR3
Title : Crystal Structure of the Processivity Clamp Loader Gamma Complex of E. coli DNA Polymerase III
Authors : Jeruzalmi, D.; O'Donnell, M.; Kuriyan, J.
Deposited on : 2001-08-10
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

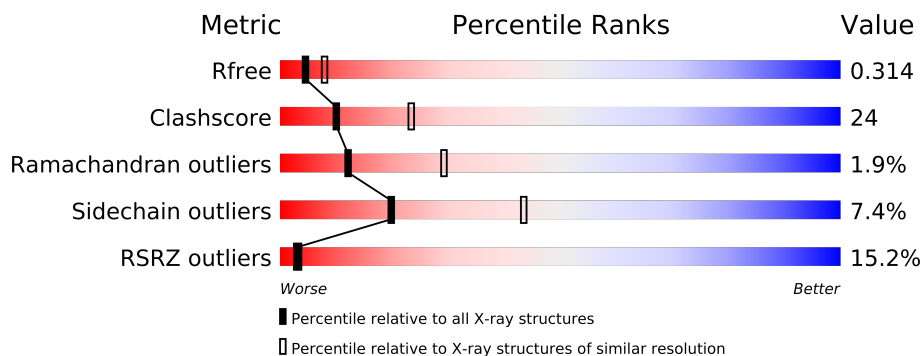
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	
1	C	373	
2	D	343	
3	E	334	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13845 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase III subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			
1	B	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
1	C	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			

- Molecule 2 is a protein called DNA polymerase III, delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	338	Total	C	N	O	S	0	0	0
			2687	1702	488	487	10			

- Molecule 3 is a protein called DNA polymerase III, delta' subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



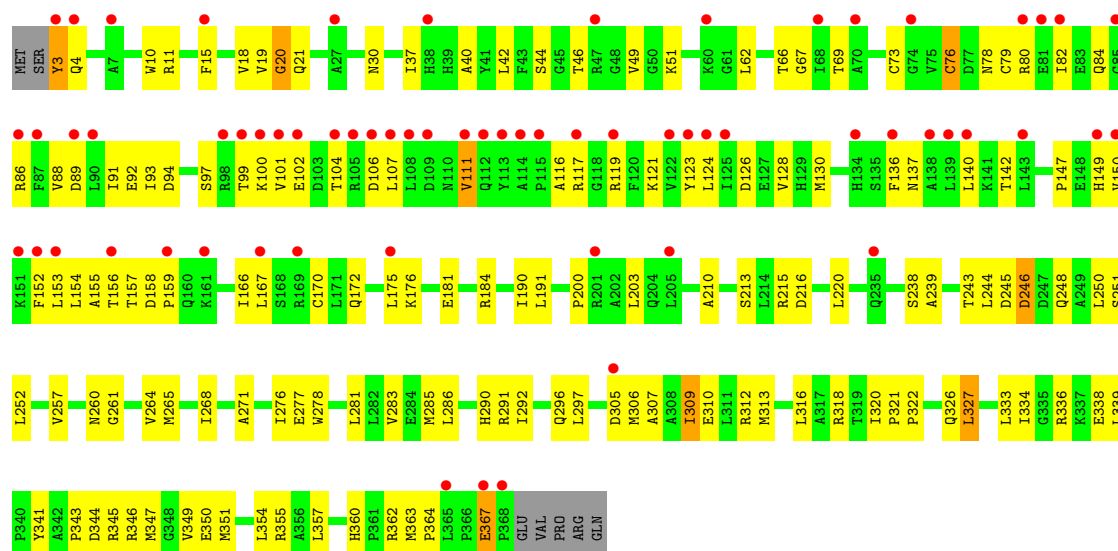
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

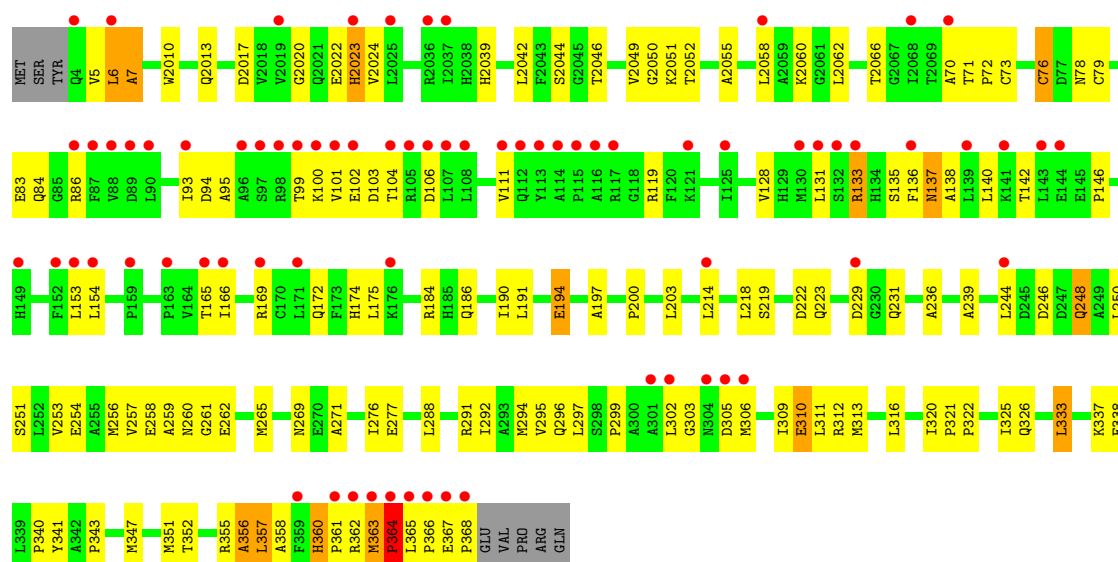
• Molecule 1: DNA polymerase III subunit gamma

Chain A: 



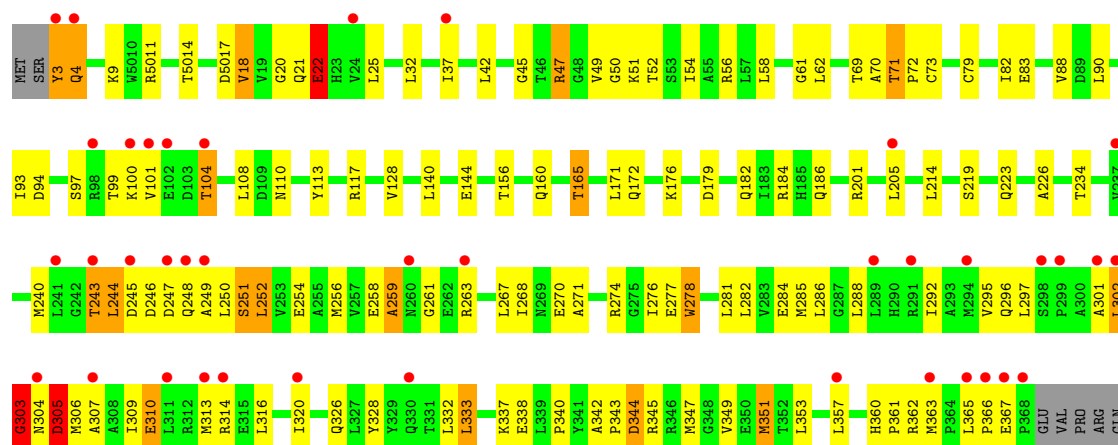
• Molecule 1: DNA polymerase III subunit gamma

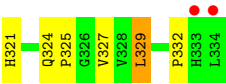
Chain B: 



• Molecule 1: DNA polymerase III subunit gamma

Chain C: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.70Å 95.86Å 285.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.70 90.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-2.70) 76.9 (90.87-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	13.60	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.268 , 0.304 0.286 , 0.314	Depositor DCC
R_{free} test set	2839 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.9	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 60122 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13845	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.48	0/2898	0.74	2/3930 (0.1%)
1	B	0.66	7/2885 (0.2%)	0.95	14/3912 (0.4%)
1	C	0.57	0/2898	0.88	10/3930 (0.3%)
2	D	0.85	8/2735 (0.3%)	0.93	10/3716 (0.3%)
3	E	0.49	0/2666	0.70	0/3639
All	All	0.62	15/14082 (0.1%)	0.85	36/19127 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	D	0	4
All	All	0	5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	315	ASP	CB-CG	29.10	2.12	1.51
1	B	133	ARG	CZ-NH2	-10.95	1.18	1.33
2	D	310	LEU	CG-CD2	-9.05	1.18	1.51
1	B	363	MET	CG-SD	8.99	2.04	1.81
1	B	363	MET	SD-CE	8.90	2.27	1.77
2	D	316	TYR	CE1-CZ	6.79	1.47	1.38
2	D	283	ARG	CB-CG	6.61	1.70	1.52
1	B	360	HIS	CA-CB	5.72	1.66	1.53
1	B	356	ALA	C-O	-5.71	1.12	1.23
2	D	316	TYR	CZ-OH	5.62	1.47	1.37
2	D	200	PRO	N-CD	-5.57	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	ARG	CZ-NH1	-5.45	1.25	1.33
2	D	316	TYR	CG-CD1	5.22	1.46	1.39
1	B	360	HIS	CG-CD2	5.18	1.44	1.35
2	D	282	ARG	CB-CG	-5.11	1.38	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	MET	CG-SD-CE	17.06	127.49	100.20
2	D	283	ARG	C-N-CA	12.38	148.31	122.30
1	C	244	LEU	CB-CG-CD2	-11.83	90.88	111.00
2	D	280	GLN	C-N-CA	11.46	150.36	121.70
1	B	133	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	B	133	ARG	NE-CZ-NH2	10.89	125.75	120.30
2	D	315	ASP	CA-CB-CG	-10.71	89.84	113.40
1	B	133	ARG	NH1-CZ-NH2	-10.47	107.88	119.40
1	B	360	HIS	N-CA-CB	10.28	129.10	110.60
2	D	283	ARG	CA-C-N	-9.34	97.53	116.20
2	D	283	ARG	NE-CZ-NH1	8.26	124.43	120.30
2	D	283	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	363	MET	CB-CG-SD	6.80	132.81	112.40
1	C	20	GLY	N-CA-C	6.75	129.97	113.10
1	C	305	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	C	302	LEU	C-N-CA	6.49	135.92	122.30
1	C	305	ASP	CB-CG-OD1	6.44	124.09	118.30
1	C	303	GLY	N-CA-C	6.36	129.01	113.10
1	A	20	GLY	N-CA-C	6.33	128.92	113.10
2	D	310	LEU	CB-CG-CD2	-6.32	100.26	111.00
1	B	7	ALA	N-CA-C	-6.14	94.43	111.00
2	D	280	GLN	O-C-N	-6.04	113.04	122.70
1	B	360	HIS	CA-CB-CG	6.00	123.81	113.60
1	B	360	HIS	CB-CA-C	-5.99	98.41	110.40
1	B	364	PRO	CA-N-CD	-5.83	103.34	111.50
1	C	245	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	A	327	LEU	CA-CB-CG	5.70	128.41	115.30
1	B	2020	GLY	N-CA-C	5.68	127.30	113.10
1	B	360	HIS	CB-CG-ND1	5.57	137.11	123.20
1	C	259	ALA	N-CA-C	5.40	125.59	111.00
2	D	282	ARG	CB-CG-CD	-5.28	97.88	111.60
1	C	243	THR	N-CA-C	5.21	125.06	111.00
1	B	303	GLY	N-CA-C	5.17	126.04	113.10
1	C	302	LEU	CA-C-N	-5.17	105.85	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ARG	N-CA-C	5.10	124.77	111.00
2	D	264	SER	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2023	HIS	Sidechain
2	D	280	GLN	Peptide
2	D	281	ASN	Mainchain
2	D	282	ARG	Mainchain
2	D	319	SER	Mainchain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2850	0	2896	158	0
1	B	2838	0	2887	195	0
1	C	2850	0	2895	133	1
2	D	2687	0	2741	146	1
3	E	2601	0	2603	100	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	5	0	0	7	0
5	B	5	0	0	2	0
5	C	5	0	0	3	0
All	All	13845	0	14022	664	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (664) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:363:MET:SD	1:B:363:MET:CG	2.04	1.45
1:C:304:ASN:ND2	2:D:234:GLN:OE1	1.61	1.30
1:B:363:MET:SD	1:B:363:MET:CE	2.27	1.21
1:C:94:ASP:H	1:C:100:LYS:NZ	1.40	1.17
2:D:315:ASP:CB	2:D:315:ASP:CG	2.12	1.16
1:B:360:HIS:HB3	1:B:363:MET:CB	1.77	1.13
1:C:304:ASN:ND2	2:D:234:GLN:CD	2.02	1.12
1:B:360:HIS:HB3	1:B:363:MET:HB2	1.11	1.09
1:C:246:ASP:HB3	1:C:274:ARG:HD3	1.38	1.06
1:C:69:THR:HG22	1:C:71:THR:H	1.15	1.05
2:D:223:MET:SD	2:D:292:ARG:HB3	1.99	1.03
1:A:351:MET:HE1	1:B:326:GLN:HE22	1.23	1.03
1:B:363:MET:HB3	1:B:364:PRO:HD2	1.42	1.01
2:D:25:GLY:HA3	2:D:139:CYS:O	1.59	1.01
1:B:355:ARG:HH21	3:E:332:PRO:HD3	1.23	0.99
2:D:119:LYS:H	2:D:119:LYS:HD3	1.26	0.99
1:C:304:ASN:ND2	2:D:234:GLN:NE2	2.10	0.98
2:D:315:ASP:HB2	2:D:318:GLN:CG	1.94	0.98
2:D:310:LEU:HD22	2:D:314:GLN:HE21	1.27	0.97
1:A:239:ALA:HB1	1:B:2023:HIS:CE1	2.00	0.97
1:B:357:LEU:HA	1:B:363:MET:SD	2.05	0.97
1:C:18:VAL:HG22	1:C:25:LEU:HD11	1.47	0.94
1:C:94:ASP:N	1:C:100:LYS:HZ3	1.63	0.94
1:A:100:LYS:CD	1:B:133:ARG:HH21	1.82	0.93
1:A:100:LYS:HD3	1:B:133:ARG:NH2	1.82	0.93
1:A:239:ALA:HB1	1:B:2023:HIS:NE2	1.83	0.92
2:D:213:THR:H	2:D:216:HIS:HD2	1.13	0.90
1:C:94:ASP:N	1:C:100:LYS:NZ	2.21	0.89
1:B:357:LEU:O	1:B:363:MET:SD	2.31	0.88
1:B:363:MET:CB	1:B:364:PRO:HD2	2.04	0.87
1:A:271:ALA:HB1	1:A:276:ILE:HD11	1.57	0.86
1:B:309:ILE:CG2	1:B:313:MET:HG2	2.05	0.86
1:B:200:PRO:HB2	1:B:305:ASP:HB2	1.57	0.86
1:A:351:MET:CE	1:B:326:GLN:HE22	1.90	0.85
1:C:179:ASP:HB3	1:C:182:GLN:HB2	1.58	0.83
3:E:8:ARG:HG3	3:E:9:PRO:HD3	1.60	0.83
2:D:55:ILE:HD13	2:D:97:LEU:HD11	1.59	0.83
2:D:312:LEU:HB2	2:D:320:VAL:HG21	1.60	0.83
1:C:3:TYR:O	1:C:4:GLN:HG3	1.79	0.82
1:A:99:THR:HG22	1:A:99:THR:O	1.78	0.81
1:B:357:LEU:HA	1:B:363:MET:CE	2.09	0.81
1:B:360:HIS:HB3	1:B:363:MET:CG	2.10	0.81
1:B:360:HIS:ND1	1:B:363:MET:CE	2.44	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:360:HIS:ND1	1:B:363:MET:HE2	1.96	0.81
2:D:315:ASP:HB2	2:D:318:GLN:HG3	1.63	0.81
1:B:253:VAL:O	1:B:257:VAL:HG23	1.80	0.81
1:A:94:ASP:O	1:A:100:LYS:HE3	1.81	0.80
3:E:58:SER:HB3	3:E:65:CYS:SG	2.21	0.80
1:B:99:THR:O	1:B:99:THR:HG22	1.81	0.80
1:C:304:ASN:ND2	2:D:234:GLN:HE22	1.77	0.80
1:A:309:ILE:HG13	1:A:313:MET:HG2	1.62	0.80
1:C:259:ALA:HB3	1:C:363:MET:HE3	1.62	0.79
1:A:97:SER:OG	1:A:100:LYS:HE3	1.83	0.79
1:A:67:GLY:HA2	1:A:119:ARG:HH12	1.47	0.79
1:B:360:HIS:CB	1:B:363:MET:CG	2.61	0.78
1:C:94:ASP:C	1:C:100:LYS:HZ1	1.86	0.78
1:B:259:ALA:HB2	1:B:363:MET:CG	2.12	0.78
1:C:93:ILE:HG23	1:C:100:LYS:HZ2	1.48	0.78
1:A:80:ARG:O	1:A:84:GLN:HG3	1.82	0.78
2:D:310:LEU:HD22	2:D:314:GLN:NE2	1.98	0.78
1:C:99:THR:HG22	1:C:99:THR:O	1.83	0.78
1:A:281:LEU:HD23	1:A:285:MET:HE2	1.66	0.78
2:D:244:VAL:HG22	2:D:312:LEU:HD21	1.64	0.78
1:A:93:ILE:CG2	1:A:100:LYS:NZ	2.47	0.78
1:A:271:ALA:CB	1:A:276:ILE:HD11	2.13	0.78
1:C:45:GLY:O	1:C:51:LYS:HE2	1.84	0.77
1:C:94:ASP:H	1:C:100:LYS:HZ3	0.81	0.77
1:B:363:MET:HB3	1:B:364:PRO:CD	2.14	0.77
1:B:244:LEU:HD21	1:B:276:ILE:HG12	1.66	0.77
1:A:128:VAL:HG11	1:A:154:LEU:HD22	1.67	0.77
1:C:4:GLN:OE1	1:C:9:LYS:HD2	1.84	0.77
2:D:300:GLN:OE1	2:D:335:PRO:CG	2.32	0.76
1:B:360:HIS:HB2	1:B:363:MET:SD	2.26	0.76
1:A:111:VAL:HG11	1:A:142:THR:HG21	1.66	0.76
2:D:222:LEU:O	2:D:223:MET:HB2	1.83	0.76
1:C:248:GLN:HG3	1:C:267:LEU:HB3	1.65	0.76
1:B:2042:LEU:HB3	1:B:172:GLN:HB3	1.67	0.76
1:B:257:VAL:O	1:B:360:HIS:HE1	1.69	0.75
1:A:276:ILE:HD13	1:A:281:LEU:HD12	1.69	0.75
1:C:271:ALA:HB1	1:C:276:ILE:HD12	1.68	0.75
1:B:2013:GLN:HE22	1:B:83:GLU:HG2	1.49	0.75
1:B:259:ALA:CB	1:B:363:MET:HG2	2.17	0.74
3:E:5:PRO:O	3:E:8:ARG:HG2	1.87	0.74
1:A:94:ASP:O	1:A:100:LYS:CE	2.35	0.74
2:D:310:LEU:HD13	2:D:314:GLN:NE2	2.01	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:357:LEU:CA	1:B:363:MET:SD	2.75	0.74
2:D:147:LEU:HB3	2:D:148:PRO:HD3	1.69	0.74
2:D:273:PHE:HB3	2:D:279:TRP:CB	2.18	0.73
1:A:156:THR:HG22	1:A:158:ASP:H	1.54	0.73
1:B:355:ARG:NH2	3:E:332:PRO:HD3	2.01	0.73
1:A:93:ILE:HG22	1:A:100:LYS:NZ	2.03	0.73
1:B:360:HIS:CG	1:B:363:MET:HG3	2.23	0.73
1:A:100:LYS:CE	1:B:133:ARG:HH21	2.00	0.73
1:C:362:ARG:HE	1:C:363:MET:HE2	1.53	0.73
1:B:358:ALA:HA	1:B:364:PRO:HG2	1.71	0.72
2:D:82:LEU:HD21	2:D:100:LEU:HD12	1.70	0.72
1:B:271:ALA:HB1	1:B:276:ILE:CD1	2.19	0.72
3:E:49:LEU:HD23	3:E:68:MET:SD	2.29	0.72
3:E:117:ALA:O	3:E:120:LEU:HD22	1.89	0.72
1:B:259:ALA:HB1	1:B:363:MET:HG2	1.72	0.72
1:B:73:CYS:O	1:B:79:CYS:SG	2.48	0.71
2:D:223:MET:SD	2:D:292:ARG:CB	2.78	0.71
2:D:300:GLN:OE1	2:D:335:PRO:HG3	1.91	0.70
1:A:326:GLN:NE2	1:C:351:MET:SD	2.65	0.70
1:C:259:ALA:CB	1:C:363:MET:HE3	2.22	0.70
1:A:360:HIS:HB3	1:A:363:MET:O	1.91	0.70
2:D:313:LYS:O	2:D:316:TYR:CZ	2.44	0.70
1:A:276:ILE:HG22	1:A:277:GLU:H	1.56	0.70
2:D:222:LEU:HD12	2:D:285:MET:HG2	1.74	0.69
1:A:94:ASP:O	1:A:100:LYS:NZ	2.25	0.69
2:D:315:ASP:CG	2:D:315:ASP:CA	2.61	0.69
2:D:213:THR:H	2:D:216:HIS:CD2	2.04	0.69
1:A:86:ARG:NH2	1:B:138:ALA:HA	2.08	0.69
1:B:338:GLU:O	1:B:341:TYR:HB2	1.93	0.69
3:E:169:GLU:O	3:E:173:VAL:HG23	1.92	0.68
2:D:55:ILE:O	2:D:85:PRO:HG3	1.93	0.68
2:D:202:VAL:O	2:D:206:VAL:HG23	1.92	0.68
1:A:73:CYS:O	1:A:79:CYS:SG	2.50	0.68
1:C:93:ILE:CG2	1:C:100:LYS:NZ	2.57	0.68
1:A:93:ILE:CG2	1:A:100:LYS:HZ3	2.06	0.68
1:C:73:CYS:O	1:C:79:CYS:SG	2.51	0.68
3:E:111:VAL:HG12	3:E:140:TRP:HB2	1.75	0.68
1:B:357:LEU:HA	1:B:363:MET:HE1	1.76	0.68
2:D:116:LYS:HB3	2:D:140:GLN:HE21	1.59	0.68
1:A:367:GLU:HG3	1:B:322:PRO:HD2	1.74	0.68
1:A:67:GLY:HA2	1:A:119:ARG:NH1	2.07	0.68
1:C:18:VAL:CG2	1:C:25:LEU:HD11	2.24	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:93:ILE:HG22	1:B:100:LYS:HZ3	1.58	0.68
2:D:308:THR:HG23	2:D:320:VAL:HG13	1.75	0.67
1:B:259:ALA:CB	1:B:363:MET:CG	2.72	0.67
1:C:93:ILE:HG23	1:C:100:LYS:NZ	2.09	0.67
1:B:254:GLU:OE2	1:B:312:ARG:HD3	1.94	0.67
1:A:11:ARG:HH22	1:B:165:THR:HG22	1.59	0.67
1:B:260:ASN:O	1:B:262:GLU:N	2.27	0.67
1:C:73:CYS:O	1:C:73:CYS:SG	2.53	0.67
1:B:223:GLN:HE21	3:E:158:ARG:HE	1.43	0.67
1:B:358:ALA:HA	1:B:364:PRO:CG	2.25	0.67
3:E:31:ALA:HB2	3:E:164:LEU:HB3	1.76	0.67
1:C:165:THR:HG23	2:D:32:GLN:HE22	1.59	0.67
1:B:309:ILE:HG22	1:B:313:MET:HG2	1.74	0.66
1:C:110:ASN:HB3	1:C:113:TYR:HD1	1.58	0.66
1:B:271:ALA:HB1	1:B:276:ILE:HD12	1.75	0.66
3:E:64:GLY:O	3:E:68:MET:HB2	1.96	0.66
3:E:74:PRO:HB3	3:E:105:ARG:HD2	1.76	0.66
1:A:181:GLU:HG2	1:A:184:ARG:HD2	1.77	0.66
1:B:93:ILE:HG22	1:B:100:LYS:NZ	2.10	0.65
1:B:347:MET:O	1:B:351:MET:HG2	1.96	0.65
2:D:274:ASP:HA	2:D:279:TRP:CE3	2.32	0.65
1:B:2013:GLN:NE2	1:B:83:GLU:HG2	2.12	0.65
3:E:8:ARG:CG	3:E:9:PRO:HD3	2.25	0.64
3:E:73:HIS:HD2	3:E:75:ASP:H	1.45	0.64
1:A:111:VAL:HG11	1:A:142:THR:CG2	2.28	0.64
2:D:48:GLU:HG3	2:D:49:GLU:N	2.13	0.64
1:B:356:ALA:O	1:B:363:MET:CE	2.45	0.64
1:B:309:ILE:HG21	1:B:313:MET:HG2	1.77	0.64
2:D:273:PHE:HB3	2:D:279:TRP:CG	2.33	0.64
1:A:261:GLY:HA3	1:B:297:LEU:HD21	1.80	0.64
1:C:268:ILE:HD11	1:C:353:LEU:CD1	2.28	0.64
1:B:360:HIS:CG	1:B:363:MET:CG	2.80	0.64
1:C:254:GLU:O	1:C:258:GLU:HG3	1.98	0.64
2:D:222:LEU:CD1	2:D:285:MET:HG2	2.29	0.63
1:A:107:LEU:HD11	1:B:133:ARG:NH1	2.14	0.63
1:A:73:CYS:SG	1:A:73:CYS:O	2.56	0.63
3:E:329:LEU:HD23	3:E:329:LEU:H	1.63	0.63
1:A:94:ASP:C	1:A:100:LYS:HZ1	2.01	0.63
1:B:6:LEU:O	1:B:218:LEU:HB3	1.98	0.63
2:D:315:ASP:HB2	2:D:318:GLN:HG2	1.80	0.62
3:E:147:GLU:HG2	3:E:147:GLU:O	1.98	0.62
1:B:100:LYS:HB2	1:B:103:ASP:OD1	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:343:PRO:HG2	1:A:347:MET:SD	2.38	0.62
2:D:24:LEU:HA	2:D:114:GLY:O	2.00	0.62
1:A:93:ILE:HG23	1:A:100:LYS:NZ	2.14	0.62
2:D:256:LEU:O	2:D:260:LEU:HG	2.00	0.62
3:E:161:LEU:H	3:E:161:LEU:HD12	1.64	0.62
1:C:328:TYR:O	1:C:332:LEU:HD23	1.99	0.62
1:A:351:MET:HA	1:A:351:MET:HE3	1.82	0.62
1:C:263:ARG:O	1:C:267:LEU:HG	2.00	0.62
1:C:271:ALA:HB1	1:C:276:ILE:CD1	2.30	0.62
1:A:239:ALA:CB	1:B:2023:HIS:CE1	2.78	0.62
1:B:337:LYS:HG3	1:B:338:GLU:N	2.12	0.62
1:C:93:ILE:CG2	1:C:100:LYS:HZ2	2.12	0.61
1:C:246:ASP:HB3	1:C:274:ARG:CD	2.24	0.61
3:E:129:LEU:HD11	3:E:158:ARG:HH11	1.64	0.61
1:B:102:GLU:HB3	1:B:106:ASP:HB2	1.80	0.61
1:A:250:LEU:HD22	1:A:309:ILE:HD12	1.82	0.61
1:C:246:ASP:CB	1:C:274:ARG:HD3	2.24	0.61
1:A:100:LYS:CD	1:B:133:ARG:NH2	2.48	0.61
1:A:86:ARG:HH21	1:B:138:ALA:HA	1.63	0.61
1:A:351:MET:CE	1:A:351:MET:HA	2.30	0.61
1:B:316:LEU:HD22	1:B:320:ILE:HD11	1.81	0.61
3:E:73:HIS:CD2	3:E:75:ASP:H	2.18	0.61
1:A:100:LYS:HD3	1:B:133:ARG:HH21	1.44	0.61
2:D:281:ASN:C	2:D:283:ARG:H	2.02	0.61
1:B:363:MET:CG	1:B:364:PRO:HD2	2.31	0.60
1:C:94:ASP:O	1:C:100:LYS:HE3	1.99	0.60
1:B:338:GLU:OE2	3:E:295:HIS:NE2	2.34	0.60
1:C:268:ILE:HD11	1:C:353:LEU:HD12	1.83	0.60
1:A:30:ASN:HD22	1:C:226:ALA:HA	1.66	0.60
1:C:51:LYS:HB2	5:C:5500:SO4:O3	2.02	0.60
1:B:70:ALA:O	1:B:72:PRO:HD3	2.01	0.60
1:C:302:LEU:HD13	1:C:310:GLU:HG2	1.84	0.60
3:E:303:VAL:HB	3:E:306:ILE:HD11	1.83	0.60
1:A:362:ARG:O	1:A:363:MET:HG3	2.02	0.60
1:C:284:GLU:O	1:C:288:LEU:HG	2.02	0.60
1:B:140:LEU:HD21	1:B:166:ILE:HG12	1.83	0.60
2:D:269:LEU:HG	2:D:273:PHE:CE1	2.37	0.59
1:A:3:TYR:O	1:A:4:GLN:HG3	2.01	0.59
1:A:88:VAL:HG11	1:A:116:ALA:HB3	1.83	0.59
1:A:152:PHE:O	1:A:153:LEU:HD23	2.02	0.59
1:A:316:LEU:HD22	1:A:320:ILE:HD11	1.84	0.59
3:E:117:ALA:HB2	3:E:143:LEU:HD12	1.83	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:292:ILE:O	1:A:296:GLN:HG3	2.02	0.59
1:C:343:PRO:HG2	1:C:347:MET:SD	2.42	0.59
1:A:21:GLN:OE1	1:A:175:LEU:HD22	2.02	0.59
1:B:246:ASP:HB2	1:B:248:GLN:HG2	1.85	0.59
1:A:93:ILE:HG22	1:A:100:LYS:HZ3	1.65	0.59
1:C:47:ARG:O	1:C:47:ARG:HG3	2.03	0.59
1:B:363:MET:CB	1:B:364:PRO:CD	2.78	0.58
1:C:205:LEU:CD1	1:C:234:THR:HG23	2.33	0.58
2:D:263:GLN:HG2	2:D:266:HIS:HD2	1.68	0.58
3:E:149:GLU:C	3:E:151:LEU:H	2.05	0.58
1:A:30:ASN:ND2	1:C:226:ALA:HA	2.18	0.58
1:A:341:TYR:HB2	1:B:333:LEU:HD11	1.84	0.58
3:E:46:ARG:CZ	3:E:68:MET:HG3	2.33	0.58
3:E:41:ILE:HG21	3:E:113:TRP:CD1	2.38	0.58
2:D:222:LEU:HD12	2:D:285:MET:SD	2.44	0.58
2:D:223:MET:HE1	2:D:292:ARG:HB2	1.86	0.58
1:A:257:VAL:HG11	1:A:320:ILE:CD1	2.34	0.58
1:B:367:GLU:HB3	1:B:368:PRO:HD2	1.86	0.58
1:C:61:GLY:HA2	1:C:72:PRO:HG3	1.85	0.58
3:E:8:ARG:HG3	3:E:9:PRO:CD	2.33	0.58
1:C:259:ALA:HB3	1:C:363:MET:CE	2.33	0.58
1:B:2058:LEU:HD23	1:B:153:LEU:HD22	1.86	0.58
1:B:360:HIS:CB	1:B:363:MET:SD	2.92	0.57
1:A:93:ILE:CG2	1:A:100:LYS:HZ2	2.17	0.57
1:B:94:ASP:O	1:B:100:LYS:HE2	2.03	0.57
1:C:282:LEU:CD2	1:C:332:LEU:HD12	2.34	0.57
2:D:10:ARG:HH12	2:D:40:GLN:NE2	2.00	0.57
2:D:279:TRP:O	2:D:279:TRP:CG	2.57	0.57
1:B:128:VAL:HG11	1:B:154:LEU:HD22	1.87	0.57
1:B:229:ASP:O	1:B:231:GLN:N	2.34	0.57
2:D:222:LEU:HD12	2:D:285:MET:CG	2.33	0.57
2:D:281:ASN:C	2:D:283:ARG:N	2.57	0.57
1:A:291:ARG:HH11	1:A:306:MET:HG3	1.69	0.57
1:C:304:ASN:OD1	1:C:305:ASP:N	2.37	0.57
1:A:49:VAL:O	5:A:1500:SO4:S	2.63	0.57
2:D:10:ARG:HH22	2:D:40:GLN:HE22	1.51	0.57
3:E:308:ARG:O	3:E:312:ILE:HG13	2.04	0.57
1:B:186:GLN:HG2	1:B:214:LEU:HD21	1.86	0.57
2:D:221:LEU:HD13	2:D:331:LEU:HD12	1.86	0.57
2:D:273:PHE:CE1	2:D:283:ARG:HG3	2.39	0.56
1:B:356:ALA:O	1:B:363:MET:HE3	2.05	0.56
1:C:328:TYR:OH	1:C:361:PRO:HD2	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:205:LEU:HD11	1:C:234:THR:HG23	1.87	0.56
1:B:296:GLN:NE2	1:B:325:ILE:HD12	2.20	0.56
2:D:170:LEU:O	2:D:173:CYS:O	2.24	0.56
1:B:194:GLU:HA	1:B:194:GLU:OE1	2.05	0.56
1:C:362:ARG:HH21	1:C:363:MET:CE	2.19	0.56
1:B:95:ALA:HA	1:B:100:LYS:HZ1	1.71	0.56
3:E:280:HIS:O	3:E:281:LEU:HD23	2.05	0.56
1:C:69:THR:HG22	1:C:71:THR:N	2.01	0.56
1:B:259:ALA:HB2	1:B:363:MET:SD	2.46	0.56
1:C:295:VAL:HG22	1:C:301:ALA:HB3	1.88	0.56
1:A:99:THR:CG2	1:A:99:THR:O	2.51	0.56
1:C:309:ILE:HG22	1:C:313:MET:HG2	1.88	0.56
1:A:156:THR:HG22	1:A:158:ASP:N	2.21	0.55
1:A:40:ALA:HB1	1:A:170:CYS:SG	2.46	0.55
1:C:362:ARG:HH21	1:C:363:MET:HE1	1.72	0.55
2:D:218:VAL:HA	2:D:221:LEU:HB2	1.88	0.55
1:C:5011:ARG:HD3	1:C:83:GLU:OE2	2.07	0.55
2:D:296:THR:HG22	2:D:299:ARG:NH1	2.21	0.55
2:D:39:ARG:NH2	2:D:50:HIS:HB3	2.21	0.55
1:B:360:HIS:HD2	1:B:361:PRO:O	1.90	0.55
2:D:308:THR:CG2	2:D:320:VAL:HG13	2.37	0.55
2:D:310:LEU:HD11	3:E:299:GLN:NE2	2.21	0.55
1:B:338:GLU:OE2	3:E:295:HIS:CE1	2.60	0.55
1:B:265:MET:HE3	3:E:257:LYS:HE2	1.89	0.55
1:B:355:ARG:NH1	3:E:287:GLN:HB3	2.22	0.55
2:D:313:LYS:O	2:D:316:TYR:CE2	2.60	0.55
1:B:259:ALA:HB2	1:B:363:MET:HG3	1.89	0.55
1:A:91:ILE:HD12	1:A:123:TYR:CE2	2.42	0.54
1:C:104:THR:O	1:C:108:LEU:HG	2.08	0.54
2:D:282:ARG:O	2:D:285:MET:HB3	2.07	0.54
1:C:297:LEU:HD23	2:D:334:LYS:O	2.06	0.54
1:C:3:TYR:O	1:C:3:TYR:CD2	2.60	0.54
1:A:97:SER:OG	1:A:100:LYS:CE	2.54	0.54
1:A:281:LEU:HD23	1:A:285:MET:CE	2.36	0.54
3:E:213:ARG:NH2	3:E:267:ASN:OD1	2.39	0.54
1:C:307:ALA:HA	1:C:310:GLU:HG3	1.89	0.54
1:B:360:HIS:CG	1:B:363:MET:CE	2.90	0.54
3:E:4:TYR:HB3	3:E:5:PRO:HD2	1.89	0.54
1:A:346:ARG:O	1:A:350:GLU:HG3	2.07	0.54
3:E:201:ALA:O	3:E:204:LEU:HB2	2.06	0.54
2:D:264:SER:O	2:D:265:ALA:HB3	2.07	0.54
1:C:49:VAL:O	5:C:5500:SO4:S	2.66	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:248:GLN:O	1:C:252:LEU:N	2.39	0.54
1:B:356:ALA:O	1:B:363:MET:HE1	2.07	0.54
2:D:1:MET:HA	2:D:134:SER:O	2.08	0.54
2:D:48:GLU:HG3	2:D:49:GLU:H	1.73	0.54
1:C:205:LEU:CD2	1:C:243:THR:HG23	2.38	0.54
1:B:244:LEU:HD11	1:B:276:ILE:HD13	1.90	0.54
2:D:271:ALA:O	2:D:275:LYS:HG2	2.07	0.53
1:C:276:ILE:HG22	1:C:277:GLU:N	2.24	0.53
2:D:262:ARG:NH2	3:E:320:GLU:OE1	2.42	0.53
1:A:94:ASP:C	1:A:100:LYS:NZ	2.62	0.53
1:B:302:LEU:HD22	1:B:306:MET:HG2	1.91	0.53
1:B:296:GLN:HE22	1:B:325:ILE:HD12	1.73	0.53
1:C:171:LEU:HA	2:D:183:GLN:HE22	1.73	0.53
2:D:119:LYS:CD	2:D:119:LYS:H	2.05	0.53
3:E:306:ILE:HG22	3:E:307:ASN:H	1.73	0.53
2:D:255:LEU:HD22	3:E:313:THR:HG21	1.91	0.53
2:D:93:ILE:HG23	2:D:97:LEU:HD13	1.91	0.53
1:B:244:LEU:HD21	1:B:276:ILE:CG1	2.37	0.53
1:A:86:ARG:HE	1:B:137:ASN:HB2	1.73	0.53
1:A:261:GLY:CA	1:B:297:LEU:HD21	2.39	0.53
1:A:307:ALA:HA	1:A:310:GLU:HB2	1.90	0.53
1:A:107:LEU:HD11	1:B:133:ARG:HH12	1.71	0.53
1:A:276:ILE:HG22	1:A:277:GLU:N	2.24	0.53
1:A:354:LEU:CD2	1:B:297:LEU:HD22	2.39	0.53
2:D:218:VAL:HG11	2:D:253:GLU:HG3	1.91	0.53
1:B:366:PRO:HB3	3:E:282:SER:HB2	1.91	0.53
1:B:259:ALA:CB	1:B:363:MET:SD	2.97	0.53
2:D:25:GLY:O	2:D:115:ASN:HA	2.08	0.53
1:B:84:GLN:HB3	1:B:86:ARG:NH2	2.24	0.53
1:B:360:HIS:HB2	1:B:363:MET:CE	2.39	0.52
1:A:191:LEU:HD12	1:A:203:LEU:HD21	1.91	0.52
1:B:271:ALA:HB1	1:B:276:ILE:HD11	1.90	0.52
2:D:309:GLU:O	2:D:313:LYS:HG3	2.09	0.52
1:A:100:LYS:HB3	1:B:133:ARG:CZ	2.39	0.52
1:B:291:ARG:HD2	1:B:306:MET:SD	2.49	0.52
2:D:273:PHE:HB3	2:D:279:TRP:HB2	1.90	0.52
3:E:268:VAL:O	3:E:271:PRO:HD3	2.09	0.52
1:B:360:HIS:O	1:B:363:MET:HB2	2.09	0.52
1:B:277:GLU:HB3	3:E:149:GLU:HG2	1.90	0.52
3:E:238:HIS:ND1	3:E:239:GLU:N	2.56	0.52
1:A:360:HIS:HD2	1:A:363:MET:H	1.57	0.52
1:A:351:MET:HE1	1:B:326:GLN:NE2	2.08	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:TRP:HB3	1:A:349:VAL:HG21	1.91	0.52
1:B:360:HIS:CG	1:B:363:MET:SD	3.02	0.52
3:E:27:LEU:O	3:E:143:LEU:N	2.39	0.52
1:B:257:VAL:HG11	1:B:320:ILE:CD1	2.40	0.52
1:B:357:LEU:C	1:B:363:MET:SD	2.88	0.52
1:B:352:THR:O	1:B:355:ARG:HB3	2.10	0.52
2:D:310:LEU:O	2:D:314:GLN:HG3	2.11	0.52
1:B:250:LEU:HD23	1:B:312:ARG:HH11	1.75	0.51
1:C:93:ILE:HG22	1:C:100:LYS:NZ	2.25	0.51
1:A:252:LEU:HD13	1:A:281:LEU:HD21	1.92	0.51
2:D:10:ARG:HH22	2:D:40:GLN:NE2	2.08	0.51
1:C:343:PRO:CG	1:C:347:MET:SD	2.99	0.51
1:A:213:SER:OG	1:A:216:ASP:HB2	2.11	0.51
1:A:334:ILE:O	1:A:338:GLU:HG3	2.09	0.51
1:A:181:GLU:HA	1:A:184:ARG:HB3	1.93	0.51
1:A:51:LYS:HE2	5:A:1500:SO4:O4	2.11	0.51
3:E:311:LEU:O	3:E:314:ASP:HB3	2.11	0.51
1:C:304:ASN:HD22	2:D:234:GLN:CD	2.03	0.51
3:E:100:LEU:HD13	3:E:139:THR:HG21	1.93	0.51
1:C:243:THR:HG22	1:C:244:LEU:N	2.26	0.51
1:C:303:GLY:HA3	1:C:306:MET:HG2	1.93	0.51
2:D:300:GLN:OE1	2:D:335:PRO:HG2	2.09	0.51
3:E:139:THR:HG22	3:E:140:TRP:N	2.26	0.51
2:D:261:LYS:HE3	2:D:295:GLN:HE21	1.76	0.51
1:A:281:LEU:CD2	1:A:285:MET:HE2	2.40	0.50
1:C:201:ARG:O	1:C:205:LEU:HG	2.11	0.50
1:A:341:TYR:HB2	1:B:333:LEU:CD1	2.41	0.50
1:B:2049:VAL:O	5:B:2500:SO4:S	2.69	0.50
2:D:294:SER:H	2:D:297:GLN:NE2	2.08	0.50
3:E:151:LEU:HD21	3:E:155:LEU:HD12	1.93	0.50
1:B:2060:LYS:HE3	1:B:79:CYS:HB3	1.93	0.50
1:C:302:LEU:HG	1:C:314:ARG:NH1	2.26	0.50
1:A:3:TYR:HB2	1:B:2039:HIS:CE1	2.46	0.50
1:B:360:HIS:CB	1:B:363:MET:CB	2.68	0.50
1:C:49:VAL:HG12	1:C:50:GLY:N	2.27	0.50
3:E:46:ARG:NH1	3:E:68:MET:HG3	2.27	0.50
1:A:89:ASP:HB3	1:A:121:LYS:HA	1.92	0.50
1:A:102:GLU:HB3	1:A:106:ASP:CB	2.41	0.50
2:D:96:GLN:O	2:D:100:LEU:HG	2.12	0.50
1:A:100:LYS:HG2	1:B:133:ARG:HE	1.77	0.50
2:D:312:LEU:HB2	2:D:320:VAL:CG2	2.35	0.50
1:A:360:HIS:CD2	1:A:362:ARG:H	2.30	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:288:LEU:O	1:B:292:ILE:HG13	2.12	0.50
1:A:107:LEU:CD1	1:B:133:ARG:HH12	2.25	0.49
3:E:312:ILE:O	3:E:316:LEU:HG	2.12	0.49
1:A:297:LEU:HD21	1:C:261:GLY:HA3	1.93	0.49
1:C:51:LYS:HE3	5:C:5500:SO4:O3	2.12	0.49
2:D:274:ASP:HA	2:D:279:TRP:CZ3	2.47	0.49
2:D:199:LEU:HB3	2:D:200:PRO:HD3	1.94	0.49
1:A:44:SER:HB2	1:A:159:PRO:HG3	1.94	0.49
1:B:2052:THR:O	1:B:2055:ALA:HB3	2.13	0.49
1:A:244:LEU:HB3	1:A:248:GLN:HB2	1.95	0.49
1:B:276:ILE:HG22	1:B:277:GLU:N	2.28	0.49
1:C:366:PRO:C	1:C:367:GLU:HG3	2.32	0.49
2:D:22:LEU:HD22	2:D:112:VAL:HB	1.94	0.49
1:A:92:GLU:HG2	1:A:124:LEU:HD23	1.94	0.49
2:D:282:ARG:HG2	2:D:285:MET:HE2	1.93	0.49
1:A:100:LYS:HE2	1:B:133:ARG:HH21	1.75	0.49
3:E:57:LYS:HG3	3:E:58:SER:H	1.78	0.49
1:C:99:THR:CG2	1:C:99:THR:O	2.53	0.49
3:E:41:ILE:HG21	3:E:113:TRP:CG	2.47	0.49
2:D:183:GLN:HA	2:D:183:GLN:HE21	1.78	0.49
2:D:27:ASP:HB3	2:D:30:LEU:HB2	1.93	0.49
1:B:236:ALA:O	1:B:239:ALA:HB3	2.12	0.49
1:C:69:THR:HG22	1:C:70:ALA:N	2.28	0.49
3:E:145:THR:HG22	3:E:147:GLU:N	2.27	0.49
2:D:296:THR:HG22	2:D:299:ARG:HH12	1.77	0.49
2:D:20:ALA:O	2:D:134:SER:HB2	2.12	0.49
1:B:360:HIS:HB2	1:B:363:MET:HE3	1.95	0.49
1:A:354:LEU:HD11	1:B:294:MET:SD	2.53	0.49
1:A:238:SER:HB2	1:A:243:THR:O	2.13	0.49
1:C:82:ILE:HG23	1:C:90:LEU:CD2	2.42	0.48
1:C:270:GLU:HG2	1:C:274:ARG:NH1	2.28	0.48
1:B:338:GLU:HA	1:B:341:TYR:CD1	2.48	0.48
1:B:140:LEU:HD22	1:B:169:ARG:CZ	2.43	0.48
1:B:302:LEU:HD11	1:B:313:MET:CB	2.43	0.48
1:C:244:LEU:HA	1:C:244:LEU:HD23	1.51	0.48
2:D:310:LEU:HD21	3:E:306:ILE:HD13	1.96	0.48
1:C:140:LEU:O	1:C:144:GLU:HG3	2.14	0.48
3:E:85:LYS:HB3	3:E:85:LYS:NZ	2.28	0.48
1:C:22:GLU:H	1:C:22:GLU:HG3	1.09	0.48
2:D:311:THR:HG23	2:D:318:GLN:CD	2.34	0.48
3:E:306:ILE:HG22	3:E:307:ASN:N	2.29	0.48
1:B:302:LEU:HD11	1:B:313:MET:HB2	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:THR:HG22	1:A:66:THR:O	2.14	0.48
2:D:10:ARG:NH2	2:D:40:GLN:HE22	2.11	0.48
1:A:101:VAL:HG12	1:A:102:GLU:HG3	1.96	0.48
3:E:57:LYS:HA	3:E:57:LYS:HD2	1.67	0.48
1:B:260:ASN:O	1:B:260:ASN:OD1	2.32	0.48
3:E:145:THR:HG22	3:E:147:GLU:H	1.78	0.47
1:C:205:LEU:HD22	1:C:243:THR:HG23	1.95	0.47
1:C:32:LEU:HD11	1:C:58:LEU:HD12	1.95	0.47
1:B:2013:GLN:HE22	1:B:83:GLU:CG	2.22	0.47
2:D:281:ASN:O	2:D:283:ARG:N	2.47	0.47
1:C:256:MET:CE	1:C:332:LEU:HD21	2.44	0.47
3:E:241:ALA:N	3:E:242:PRO:HD2	2.29	0.47
2:D:48:GLU:CG	2:D:49:GLU:N	2.76	0.47
1:A:291:ARG:NH1	1:A:306:MET:HG3	2.29	0.47
1:A:216:ASP:O	1:A:220:LEU:HG	2.15	0.47
2:D:98:LEU:O	2:D:101:THR:HG22	2.14	0.47
1:B:257:VAL:HG11	1:B:320:ILE:HD13	1.95	0.47
2:D:310:LEU:HD13	2:D:314:GLN:HE22	1.77	0.47
1:C:333:LEU:CD1	1:C:337:LYS:HE3	2.45	0.47
1:C:292:ILE:O	1:C:296:GLN:HG3	2.14	0.47
1:B:2024:VAL:HG11	1:B:175:LEU:HD21	1.96	0.47
1:C:94:ASP:N	1:C:100:LYS:HZ1	2.07	0.47
1:A:271:ALA:HB1	1:A:276:ILE:CD1	2.36	0.47
1:A:316:LEU:HB3	1:A:320:ILE:HD12	1.96	0.47
1:C:286:LEU:HD11	1:C:333:LEU:HA	1.96	0.47
1:A:126:ASP:HA	1:A:155:ALA:HB3	1.96	0.47
1:B:244:LEU:HD11	1:B:276:ILE:CG2	2.45	0.47
1:B:2044:SER:OG	1:B:174:HIS:HA	2.15	0.47
3:E:227:GLY:O	3:E:229:TRP:HD1	1.98	0.47
1:B:256:MET:HA	1:B:357:LEU:HD11	1.97	0.47
1:C:50:GLY:O	1:C:54:ILE:HG13	2.15	0.47
2:D:60:ASP:O	2:D:64:ILE:HD12	2.15	0.47
2:D:263:GLN:HB2	2:D:272:LEU:HD21	1.97	0.47
1:A:147:PRO:HG2	1:A:150:VAL:HB	1.96	0.46
3:E:241:ALA:O	3:E:245:LEU:HD22	2.14	0.46
1:C:362:ARG:HE	1:C:363:MET:CE	2.24	0.46
1:B:343:PRO:HG3	1:B:347:MET:SD	2.56	0.46
1:B:246:ASP:HB2	1:B:248:GLN:CG	2.45	0.46
1:A:149:HIS:H	1:A:149:HIS:CD2	2.34	0.46
2:D:311:THR:HG23	2:D:318:GLN:OE1	2.15	0.46
1:A:93:ILE:HG23	1:A:100:LYS:HZ3	1.76	0.46
1:B:165:THR:O	1:B:169:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:284:GLY:O	2:D:288:GLU:HB2	2.16	0.46
1:B:316:LEU:HD22	1:B:320:ILE:CD1	2.45	0.46
2:D:315:ASP:CB	2:D:318:GLN:HG2	2.45	0.46
1:A:246:ASP:O	1:A:250:LEU:HB2	2.16	0.46
1:B:2042:LEU:HB3	1:B:172:GLN:CB	2.42	0.46
1:B:338:GLU:HA	1:B:341:TYR:HD1	1.81	0.46
2:D:251:GLN:OE1	3:E:307:ASN:ND2	2.49	0.46
2:D:213:THR:N	2:D:216:HIS:HD2	1.96	0.46
1:A:257:VAL:HG11	1:A:320:ILE:HD13	1.97	0.46
2:D:263:GLN:OE1	2:D:272:LEU:HD11	2.15	0.46
1:B:2051:LYS:HE3	1:B:2051:LYS:HB2	1.76	0.46
3:E:95:GLU:O	3:E:99:LYS:HB2	2.16	0.46
1:B:2042:LEU:HD12	1:B:172:GLN:OE1	2.16	0.46
1:C:94:ASP:O	1:C:100:LYS:CE	2.63	0.46
2:D:315:ASP:HB2	2:D:318:GLN:CD	2.36	0.46
2:D:222:LEU:CD1	2:D:285:MET:SD	3.04	0.46
1:A:257:VAL:O	1:A:360:HIS:HE1	1.99	0.46
3:E:257:LYS:HB3	3:E:262:ALA:HB3	1.98	0.46
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.54	0.46
1:B:338:GLU:CD	3:E:295:HIS:HE2	2.18	0.46
1:A:21:GLN:HE22	1:A:49:VAL:HG13	1.81	0.46
1:C:56:ARG:NH1	1:C:82:ILE:O	2.49	0.46
1:C:186:GLN:HG2	1:C:214:LEU:HD21	1.98	0.46
2:D:174:TYR:CE2	2:D:211:HIS:CE1	3.04	0.46
1:B:291:ARG:O	1:B:295:VAL:HG23	2.16	0.45
3:E:27:LEU:CD2	3:E:29:ILE:HD11	2.46	0.45
1:A:51:LYS:HB2	1:A:51:LYS:HE3	1.77	0.45
3:E:282:SER:OG	3:E:285:ARG:HB2	2.16	0.45
1:A:260:ASN:OD1	1:A:260:ASN:O	2.35	0.45
1:A:252:LEU:CD1	1:A:281:LEU:HD21	2.47	0.45
1:B:197:ALA:HB3	1:B:231:GLN:HG2	1.98	0.45
1:A:333:LEU:CD2	1:C:338:GLU:HB3	2.46	0.45
1:C:219:SER:O	1:C:223:GLN:HG3	2.17	0.45
2:D:247:LEU:HD11	2:D:308:THR:HG22	1.98	0.45
2:D:279:TRP:O	2:D:279:TRP:CD2	2.69	0.45
1:A:265:MET:HE2	1:B:294:MET:SD	2.56	0.45
1:C:344:ASP:O	1:C:347:MET:HB3	2.16	0.45
2:D:19:ALA:CB	2:D:133:ARG:HD3	2.45	0.45
1:B:2051:LYS:HB2	5:B:2500:SO4:O3	2.17	0.45
2:D:312:LEU:O	2:D:312:LEU:HG	2.15	0.45
1:A:215:ARG:NH2	5:A:1500:SO4:O2	2.50	0.45
3:E:14:LEU:HD13	3:E:44:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:222:LEU:HD11	2:D:285:MET:CE	2.47	0.45
2:D:48:GLU:CG	2:D:49:GLU:H	2.30	0.45
3:E:51:GLN:HB2	3:E:62:CYS:HB2	1.98	0.45
2:D:315:ASP:HB2	2:D:318:GLN:NE2	2.31	0.45
1:C:270:GLU:HG2	1:C:274:ARG:CZ	2.46	0.45
1:A:73:CYS:SG	1:A:76:CYS:HB3	2.56	0.45
1:B:361:PRO:O	1:B:362:ARG:HB2	2.15	0.45
3:E:299:GLN:HE21	3:E:311:LEU:HD21	1.82	0.45
3:E:27:LEU:HG	3:E:29:ILE:CD1	2.47	0.45
3:E:253:MET:O	3:E:256:LEU:N	2.49	0.45
2:D:198:THR:HB	2:D:200:PRO:HD2	1.98	0.45
1:B:258:GLU:O	1:B:259:ALA:HB3	2.17	0.45
2:D:221:LEU:HD23	2:D:221:LEU:HA	1.47	0.45
2:D:27:ASP:OD2	2:D:178:LEU:HD12	2.17	0.45
2:D:225:LYS:HE3	2:D:227:LYS:HD2	1.99	0.45
2:D:298:LEU:O	2:D:302:VAL:HG23	2.16	0.45
1:B:2066:THR:O	1:B:2066:THR:HG22	2.17	0.45
1:C:248:GLN:O	1:C:252:LEU:HB2	2.17	0.44
1:A:86:ARG:HH21	1:B:138:ALA:CA	2.27	0.44
1:B:140:LEU:HD11	1:B:165:THR:HB	1.99	0.44
3:E:30:GLN:HA	3:E:145:THR:O	2.17	0.44
1:A:21:GLN:NE2	1:A:176:LYS:O	2.49	0.44
1:B:2062:LEU:O	1:B:119:ARG:HD2	2.18	0.44
1:B:142:THR:O	1:B:146:PRO:N	2.50	0.44
1:C:316:LEU:HD22	1:C:320:ILE:HD11	1.98	0.44
2:D:315:ASP:H	2:D:318:GLN:HE21	1.65	0.44
2:D:25:GLY:N	2:D:114:GLY:O	2.41	0.44
3:E:149:GLU:C	3:E:151:LEU:N	2.71	0.44
1:C:307:ALA:HA	1:C:310:GLU:CG	2.47	0.44
1:A:102:GLU:HB3	1:A:106:ASP:HB2	1.99	0.44
1:A:147:PRO:HB2	1:A:149:HIS:CD2	2.52	0.44
1:A:37:ILE:HD12	1:A:62:LEU:HD21	1.98	0.44
3:E:324:GLN:HA	3:E:325:PRO:HD3	1.86	0.44
1:C:42:LEU:HD23	1:C:172:GLN:HG2	1.99	0.44
1:B:343:PRO:HB2	3:E:246:HIS:ND1	2.33	0.44
2:D:57:PRO:HB3	2:D:90:ASN:ND2	2.33	0.44
1:B:257:VAL:O	1:B:257:VAL:HG12	2.17	0.44
1:A:215:ARG:CZ	5:A:1500:SO4:O1	2.65	0.44
1:B:2010:TRP:CE2	1:B:190:ILE:HG23	2.53	0.44
1:C:250:LEU:HD13	1:C:288:LEU:HD13	2.00	0.44
1:C:250:LEU:HD22	1:C:309:ILE:CG2	2.48	0.44
1:B:229:ASP:C	1:B:231:GLN:N	2.71	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:131:LEU:HB2	1:B:136:PHE:CD1	2.52	0.44
1:A:42:LEU:HD12	1:A:154:LEU:HB2	2.00	0.44
1:C:248:GLN:HA	1:C:251:SER:OG	2.17	0.44
1:A:245:ASP:HB2	1:A:248:GLN:HG3	1.99	0.44
2:D:315:ASP:CB	2:D:318:GLN:CG	2.82	0.44
1:C:360:HIS:CD2	1:C:361:PRO:HD2	2.52	0.44
1:B:135:SER:O	1:B:138:ALA:HB3	2.17	0.44
1:A:290:HIS:CE1	1:C:347:MET:HG3	2.53	0.44
1:B:191:LEU:HD12	1:B:203:LEU:HD21	1.99	0.44
1:B:94:ASP:O	1:B:100:LYS:CE	2.65	0.43
3:E:30:GLN:HG3	3:E:30:GLN:O	2.18	0.43
1:A:167:LEU:HB3	1:A:172:GLN:NE2	2.33	0.43
2:D:56:ASP:HB3	2:D:58:ASN:H	1.83	0.43
2:D:100:LEU:O	2:D:103:LEU:HB3	2.18	0.43
1:C:326:GLN:CD	2:D:338:ASP:OD2	2.56	0.43
2:D:3:ARG:HG2	2:D:136:GLN:NE2	2.33	0.43
3:E:117:ALA:HB2	3:E:143:LEU:CD1	2.47	0.43
1:C:243:THR:CG2	1:C:244:LEU:N	2.81	0.43
1:C:104:THR:HG22	1:C:108:LEU:HG	1.99	0.43
2:D:325:GLU:O	2:D:329:LEU:HG	2.18	0.43
1:C:340:PRO:HB3	1:C:345:ARG:HH21	1.83	0.43
1:C:21:GLN:HE22	1:C:49:VAL:CG1	2.32	0.43
1:C:244:LEU:HD23	1:C:247:ASP:OD2	2.17	0.43
2:D:50:HIS:O	2:D:51:HIS:CD2	2.72	0.43
1:C:42:LEU:HD11	1:C:156:THR:HG22	2.01	0.43
3:E:7:LEU:HD22	3:E:40:LEU:HB2	2.00	0.43
1:C:307:ALA:HA	1:C:310:GLU:CD	2.38	0.43
1:A:345:ARG:O	1:A:349:VAL:HG23	2.19	0.43
1:A:10:TRP:CZ2	1:A:190:ILE:HG23	2.54	0.43
1:A:264:VAL:O	1:A:268:ILE:HG13	2.18	0.43
1:B:358:ALA:C	1:B:360:HIS:H	2.22	0.43
3:E:51:GLN:HG2	3:E:62:CYS:SG	2.58	0.43
3:E:165:ALA:HA	3:E:166:PRO:HD3	1.89	0.43
2:D:29:LEU:O	2:D:33:GLU:HG3	2.19	0.43
1:A:94:ASP:N	1:A:100:LYS:HZ3	2.17	0.43
1:B:337:LYS:O	1:B:340:PRO:HD2	2.19	0.43
1:B:269:ASN:ND2	3:E:264:GLN:HG3	2.34	0.43
2:D:191:LEU:O	2:D:193:PRO:HD3	2.18	0.43
2:D:119:LYS:HD3	2:D:119:LYS:N	2.11	0.43
1:B:265:MET:CE	3:E:257:LYS:HE2	2.49	0.43
1:C:278:TRP:CE3	1:C:349:VAL:HG21	2.53	0.42
1:B:5:VAL:HG13	1:B:222:ASP:CG	2.38	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:321:PRO:HA	1:B:322:PRO:HD2	1.92	0.42
1:C:37:ILE:HG12	1:C:62:LEU:HD21	2.02	0.42
1:C:276:ILE:CG2	1:C:277:GLU:N	2.82	0.42
1:B:131:LEU:HB2	1:B:136:PHE:HD1	1.85	0.42
1:A:136:PHE:CZ	1:A:166:ILE:HD12	2.54	0.42
3:E:245:LEU:HB2	3:E:297:ARG:HG3	2.01	0.42
1:B:76:CYS:SG	1:B:78:ASN:HB2	2.59	0.42
1:C:248:GLN:HA	1:C:251:SER:HG	1.85	0.42
1:A:156:THR:HG22	1:A:157:THR:N	2.34	0.42
1:B:347:MET:O	1:B:351:MET:CG	2.65	0.42
1:C:104:THR:HG22	1:C:108:LEU:CD1	2.50	0.42
1:A:333:LEU:O	1:A:336:ARG:N	2.49	0.42
3:E:92:ALA:O	3:E:96:VAL:HG23	2.19	0.42
1:B:271:ALA:O	1:B:276:ILE:HG13	2.20	0.42
1:A:362:ARG:C	1:A:363:MET:HG3	2.40	0.42
2:D:311:THR:O	2:D:318:GLN:NE2	2.53	0.42
1:A:147:PRO:HB2	1:A:149:HIS:NE2	2.35	0.42
1:A:333:LEU:HD22	1:C:338:GLU:HB3	2.02	0.42
1:B:119:ARG:H	1:B:119:ARG:HG3	1.65	0.42
3:E:18:TYR:HB3	3:E:48:LEU:HD21	2.00	0.42
2:D:243:PRO:HG2	2:D:244:VAL:H	1.85	0.42
1:C:342:ALA:HB1	1:C:343:PRO:HD2	2.01	0.42
2:D:264:SER:O	2:D:265:ALA:CB	2.68	0.42
1:A:200:PRO:HG2	1:A:305:ASP:CG	2.40	0.42
1:B:244:LEU:CD1	1:B:276:ILE:HD13	2.48	0.41
1:B:351:MET:SD	3:E:290:LEU:HD13	2.59	0.41
1:A:210:ALA:HB1	1:A:213:SER:OG	2.20	0.41
2:D:142:PRO:CD	2:D:178:LEU:HD11	2.50	0.41
2:D:79:THR:HG22	2:D:80:LEU:N	2.34	0.41
3:E:197:SER:HA	3:E:198:PRO:HD3	1.87	0.41
2:D:64:ILE:HG12	2:D:96:GLN:HB3	2.02	0.41
1:A:215:ARG:NH2	5:A:1500:SO4:O1	2.53	0.41
1:B:351:MET:SD	3:E:290:LEU:HD22	2.60	0.41
1:A:320:ILE:HA	1:A:321:PRO:HD3	1.89	0.41
2:D:4:LEU:CD1	2:D:137:VAL:HG22	2.50	0.41
3:E:225:PRO:HB3	3:E:276:GLU:OE2	2.20	0.41
1:A:78:ASN:O	1:A:82:ILE:HG13	2.20	0.41
1:B:360:HIS:CB	1:B:363:MET:HE3	2.50	0.41
1:B:244:LEU:HD11	1:B:276:ILE:HG21	2.02	0.41
1:A:215:ARG:NH2	5:A:1500:SO4:S	2.94	0.41
1:C:140:LEU:HA	1:C:140:LEU:HD23	1.84	0.41
1:A:18:VAL:HG12	1:A:19:VAL:N	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:283:VAL:HA	1:A:286:LEU:HD12	2.03	0.41
1:A:250:LEU:HD23	1:A:312:ARG:CZ	2.51	0.41
1:B:343:PRO:CG	1:B:347:MET:SD	3.09	0.41
3:E:329:LEU:HD23	3:E:329:LEU:N	2.34	0.41
1:C:281:LEU:O	1:C:285:MET:HG3	2.20	0.41
2:D:310:LEU:HD23	2:D:310:LEU:HA	1.61	0.41
1:B:302:LEU:HD13	1:B:310:GLU:HA	2.03	0.41
1:A:362:ARG:HA	1:A:362:ARG:HD3	1.95	0.41
3:E:239:GLU:HA	3:E:308:ARG:CZ	2.51	0.41
3:E:121:THR:O	3:E:124:ALA:HB3	2.21	0.41
3:E:170:GLN:HG2	3:E:170:GLN:H	1.65	0.41
2:D:310:LEU:HB3	2:D:314:GLN:NE2	2.35	0.41
2:D:270:ARG:HG2	2:D:283:ARG:NH2	2.36	0.40
1:A:257:VAL:HG12	1:A:257:VAL:O	2.21	0.40
3:E:73:HIS:HA	3:E:74:PRO:HD3	1.77	0.40
3:E:321:HIS:O	3:E:327:VAL:HG21	2.22	0.40
1:A:276:ILE:H	1:A:276:ILE:HG13	1.66	0.40
2:D:281:ASN:O	2:D:281:ASN:OD1	2.40	0.40
3:E:73:HIS:CE1	3:E:106:LEU:HD22	2.56	0.40
1:B:311:LEU:HA	1:B:311:LEU:HD12	1.88	0.40
3:E:256:LEU:HD12	3:E:290:LEU:HD12	2.03	0.40
1:B:297:LEU:HD12	1:B:297:LEU:HA	1.90	0.40
2:D:213:THR:C	2:D:215:PHE:N	2.75	0.40
1:B:250:LEU:CD2	1:B:309:ILE:HG23	2.51	0.40
2:D:39:ARG:CZ	2:D:50:HIS:HB3	2.51	0.40
1:C:82:ILE:HG23	1:C:90:LEU:HD23	2.03	0.40
3:E:163:TYR:CE2	3:E:165:ALA:HB2	2.57	0.40
1:A:137:ASN:HA	1:A:140:LEU:HD12	2.02	0.40
1:A:49:VAL:O	5:A:1500:SO4:O1	2.40	0.40
1:B:365:LEU:HB3	1:B:366:PRO:HD2	2.04	0.40
1:C:32:LEU:HA	1:C:32:LEU:HD23	1.94	0.40
3:E:171:TYR:CD2	3:E:171:TYR:N	2.88	0.40
1:A:322:PRO:HG3	1:C:365:LEU:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:117:ARG:NH2	2:D:281:ASN:ND2[4_486]	1.70	0.50

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/373 (98%)	335 (92%)	23 (6%)	6 (2%)	14	35
1	B	363/373 (97%)	325 (90%)	28 (8%)	10 (3%)	8	18
1	C	364/373 (98%)	334 (92%)	22 (6%)	8 (2%)	10	25
2	D	336/343 (98%)	307 (91%)	22 (6%)	7 (2%)	11	27
3	E	332/334 (99%)	301 (91%)	29 (9%)	2 (1%)	33	66
All	All	1759/1796 (98%)	1602 (91%)	124 (7%)	33 (2%)	12	29

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	GLY
1	A	104	THR
1	A	111	VAL
1	A	364	PRO
1	B	2022	GLU
1	B	104	THR
1	B	261	GLY
1	B	310	GLU
1	C	310	GLU
2	D	279	TRP
1	B	2050	GLY
1	C	104	THR
1	C	303	GLY
2	D	131	ALA
2	D	282	ARG
1	B	111	VAL
1	C	4	GLN
2	D	46	GLY
2	D	269	LEU
3	E	62	CYS
1	C	249	ALA
2	D	125	ALA
3	E	150	ARG

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Mol	Chain	Res	Type
1	A	339	LEU
1	B	7	ALA
1	B	364	PRO
1	C	22	GLU
1	C	278	TRP
1	A	246	ASP
1	B	101	VAL
1	B	299	PRO
2	D	317	GLY
1	C	101	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/310 (98%)	288 (95%)	15 (5%)	34	66
1	B	302/310 (97%)	289 (96%)	13 (4%)	40	72
1	C	303/310 (98%)	280 (92%)	23 (8%)	19	41
2	D	287/291 (99%)	261 (91%)	26 (9%)	14	30
3	E	270/270 (100%)	239 (88%)	31 (12%)	8	19
All	All	1465/1491 (98%)	1357 (93%)	108 (7%)	20	43

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	15	PHE
1	A	46	THR
1	A	69	THR
1	A	76	CYS
1	A	117	ARG
1	A	130	MET
1	A	251	SER
1	A	309	ILE
1	A	318	ARG
1	A	327	LEU

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Mol	Chain	Res	Type
1	A	344	ASP
1	A	355	ARG
1	A	357	LEU
1	A	367	GLU
1	B	6	LEU
1	B	2017	ASP
1	B	2046	THR
1	B	71	THR
1	B	76	CYS
1	B	137	ASN
1	B	184	ARG
1	B	194	GLU
1	B	219	SER
1	B	248	GLN
1	B	251	SER
1	B	333	LEU
1	B	357	LEU
1	C	3	TYR
1	C	5014	THR
1	C	5017	ASP
1	C	18	VAL
1	C	22	GLU
1	C	47	ARG
1	C	52	THR
1	C	71	THR
1	C	88	VAL
1	C	97	SER
1	C	128	VAL
1	C	160	GLN
1	C	165	THR
1	C	176	LYS
1	C	184	ARG
1	C	240	MET
1	C	251	SER
1	C	252	LEU
1	C	305	ASP
1	C	333	LEU
1	C	344	ASP
1	C	351	MET
1	C	357	LEU
2	D	40	GLN
2	D	54	SER

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Mol	Chain	Res	Type
2	D	84	LEU
2	D	101	THR
2	D	109	LEU
2	D	113	ARG
2	D	115	ASN
2	D	119	LYS
2	D	133	ARG
2	D	143	GLU
2	D	160	LEU
2	D	162	LEU
2	D	183	GLN
2	D	198	THR
2	D	200	PRO
2	D	208	ASP
2	D	215	PHE
2	D	223	MET
2	D	228	ARG
2	D	230	LEU
2	D	266	HIS
2	D	279	TRP
2	D	283	ARG
2	D	292	ARG
2	D	305	LEU
2	D	330	LEU
3	E	3	TRP
3	E	13	LYS
3	E	46	ARG
3	E	68	MET
3	E	91	ASP
3	E	110	LYS
3	E	120	LEU
3	E	147	GLU
3	E	149	GLU
3	E	154	THR
3	E	158	ARG
3	E	159	CYS
3	E	170	GLN
3	E	175	TRP
3	E	185	ASP
3	E	202	LEU
3	E	206	GLN
3	E	216	LEU

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Mol	Chain	Res	Type
3	E	220	LEU
3	E	237	ASN
3	E	245	LEU
3	E	252	LEU
3	E	256	LEU
3	E	277	LEU
3	E	285	ARG
3	E	290	LEU
3	E	292	ASP
3	E	299	GLN
3	E	310	LEU
3	E	315	LEU
3	E	329	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	198	HIS
1	A	360	HIS
1	B	2023	HIS
1	B	198	HIS
1	B	223	GLN
1	B	248	GLN
1	B	326	GLN
1	C	198	HIS
1	C	360	HIS
2	D	32	GLN
2	D	40	GLN
2	D	51	HIS
2	D	94	ASN
2	D	105	HIS
2	D	136	GLN
2	D	183	GLN
2	D	204	GLN
2	D	211	HIS
2	D	216	HIS
2	D	266	HIS
2	D	276	HIS
2	D	295	GLN
2	D	297	GLN
2	D	314	GLN

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Mol	Chain	Res	Type
2	D	318	GLN
3	E	73	HIS
3	E	237	ASN
3	E	280	HIS
3	E	299	GLN
3	E	307	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	A	1500	-	4,4,4	3.53	2 (50%)	6,6,6	0.93	0
5	SO4	B	2500	-	4,4,4	3.46	2 (50%)	6,6,6	0.94	0
5	SO4	C	5500	-	4,4,4	3.49	2 (50%)	6,6,6	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	1500	-	-	0/0/0/0	0/0/0/0
5	SO4	B	2500	-	-	0/0/0/0	0/0/0/0
5	SO4	C	5500	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1500	SO4	O3-S	-5.40	1.28	1.47
5	C	5500	SO4	O3-S	-5.24	1.29	1.47
5	B	2500	SO4	O3-S	-4.96	1.30	1.47
5	B	2500	SO4	O1-S	4.77	1.62	1.47
5	C	5500	SO4	O1-S	4.55	1.61	1.47
5	A	1500	SO4	O1-S	4.34	1.61	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	366/373 (98%)	1.10	65 (17%) 2 2	32, 76, 152, 173	0
1	B	365/373 (97%)	1.42	74 (20%) 1 2	27, 75, 159, 190	0
1	C	366/373 (98%)	0.95	39 (10%) 6 6	27, 62, 129, 156	0
2	D	338/343 (98%)	0.87	34 (10%) 7 8	38, 69, 121, 142	0
3	E	334/334 (100%)	1.22	58 (17%) 2 2	30, 67, 156, 161	0
All	All	1769/1796 (98%)	1.12	270 (15%) 3 3	27, 69, 151, 190	0

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	PRO	19.4
1	B	365	LEU	15.6
1	B	364	PRO	14.1
1	B	359	PHE	12.5
1	B	366	PRO	12.2
1	B	367	GLU	10.8
3	E	108	GLY	10.1
1	A	104	THR	9.6
1	B	100	LYS	8.5
1	A	152	PHE	8.3
1	A	101	VAL	8.2
3	E	101	ASN	7.7
3	E	103	HIS	7.6
1	C	241	LEU	7.4
1	A	108	LEU	7.3
1	B	101	VAL	7.3
3	E	55	GLY	7.3
1	A	3	TYR	7.2
2	D	333	HIS	7.1
1	B	108	LEU	7.0

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Mol	Chain	Res	Type	RSRZ
2	D	316	TYR	7.0
1	B	136	PHE	6.6
1	B	98	ARG	6.2
2	D	338	ASP	6.2
3	E	82	GLU	6.1
1	B	2023	HIS	6.0
1	A	368	PRO	5.9
3	E	109	ALA	5.9
1	B	104	THR	5.8
1	C	363	MET	5.7
3	E	61	HIS	5.7
1	C	302	LEU	5.6
1	B	363	MET	5.5
1	C	248	GLN	5.4
3	E	54	GLN	5.4
3	E	333	HIS	5.4
1	B	99	THR	5.4
3	E	77	TYR	5.4
2	D	317	GLY	5.3
1	C	294	MET	5.2
1	B	2068	ILE	5.1
3	E	76	TYR	5.1
1	A	102	GLU	5.1
3	E	146	ARG	5.1
3	E	74	PRO	4.9
3	E	83	LYS	4.9
1	A	86	ARG	4.9
1	A	112	GLN	4.9
3	E	112	VAL	4.7
2	D	277	ARG	4.7
1	B	361	PRO	4.7
1	B	90	LEU	4.7
3	E	79	LEU	4.6
2	D	275	LYS	4.6
1	A	153	LEU	4.6
1	C	247	ASP	4.6
1	B	133	ARG	4.6
1	A	122	VAL	4.5
1	A	74	GLY	4.5
1	B	107	LEU	4.5
1	A	124	LEU	4.3
1	B	132	SER	4.3

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Mol	Chain	Res	Type	RSRZ
2	D	279	TRP	4.3
1	B	113	TYR	4.3
1	B	86	ARG	4.3
3	E	127	ALA	4.2
1	B	362	ARG	4.1
1	A	138	ALA	4.1
1	B	302	LEU	4.0
1	C	366	PRO	4.0
1	B	111	VAL	4.0
1	A	111	VAL	4.0
1	B	117	ARG	3.9
2	D	318	GLN	3.9
3	E	102	GLU	3.9
1	B	244	LEU	3.9
3	E	63	ARG	3.9
1	B	105	ARG	3.9
3	E	95	GLU	3.8
1	B	6	LEU	3.8
1	B	97	SER	3.8
1	B	115	PRO	3.8
1	A	81	GLU	3.8
1	A	100	LYS	3.8
1	A	367	GLU	3.8
1	B	112	GLN	3.7
1	B	125	ILE	3.7
1	C	311	LEU	3.7
2	D	283	ARG	3.7
3	E	46	ARG	3.7
1	C	301	ALA	3.7
3	E	84	GLY	3.7
1	B	93	ILE	3.7
1	B	70	ALA	3.6
1	B	229	ASP	3.6
3	E	20	ALA	3.6
1	B	102	GLU	3.6
3	E	51	GLN	3.6
1	C	245	ASP	3.6
1	A	150	VAL	3.6
2	D	336	LEU	3.6
3	E	334	LEU	3.6
1	C	313	MET	3.6
1	B	87	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	134	HIS	3.5
3	E	150	ARG	3.5
1	A	151	LYS	3.5
3	E	85	LYS	3.5
2	D	2	ILE	3.5
1	C	101	VAL	3.4
1	B	149	HIS	3.4
3	E	53	PRO	3.4
3	E	106	LEU	3.4
3	E	126	ASN	3.4
3	E	132	LEU	3.4
1	C	299	PRO	3.3
1	A	4	GLN	3.2
2	D	233	LEU	3.2
1	B	306	MET	3.2
1	A	47	ARG	3.2
2	D	330	LEU	3.2
2	D	227	LYS	3.2
1	C	291	ARG	3.2
1	A	107	LEU	3.2
1	C	100	LYS	3.2
1	B	116	ALA	3.1
1	C	104	THR	3.1
1	C	4	GLN	3.1
1	B	2036	ARG	3.1
1	A	161	LYS	3.1
1	A	70	ALA	3.1
3	E	56	HIS	3.1
1	A	365	LEU	3.0
1	C	298	SER	3.0
3	E	81	PRO	3.0
3	E	58	SER	3.0
1	B	131	LEU	3.0
2	D	320	VAL	2.9
1	B	166	ILE	2.9
1	C	367	GLU	2.9
1	A	98	ARG	2.9
3	E	66	GLN	2.9
1	B	152	PHE	2.9
3	E	224	VAL	2.9
1	A	136	PHE	2.8
1	A	175	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	365	LEU	2.8
1	C	249	ALA	2.8
1	A	117	ARG	2.8
2	D	236	LEU	2.8
3	E	133	GLU	2.8
1	B	176	LYS	2.8
3	E	123	ALA	2.8
3	E	129	LEU	2.8
1	C	263	ARG	2.8
2	D	319	SER	2.8
1	B	154	LEU	2.8
1	A	99	THR	2.8
3	E	42	TYR	2.8
1	B	106	ASP	2.8
2	D	334	LYS	2.8
1	B	2025	LEU	2.7
1	B	2058	LEU	2.7
1	C	205	LEU	2.7
1	A	159	PRO	2.7
3	E	60	GLY	2.7
3	E	113	TRP	2.7
1	B	114	ALA	2.7
1	B	130	MET	2.7
1	A	15	PHE	2.7
1	A	113	TYR	2.7
3	E	71	GLY	2.7
1	B	153	LEU	2.7
1	A	235	GLN	2.7
1	A	38	HIS	2.7
1	B	169	ARG	2.7
3	E	124	ALA	2.7
1	C	314	ARG	2.7
1	A	89	ASP	2.6
1	A	169	ARG	2.6
3	E	44	LEU	2.6
1	A	115	PRO	2.6
1	B	4	GLN	2.6
2	D	270	ARG	2.6
1	A	140	LEU	2.6
1	A	143	LEU	2.6
3	E	110	LYS	2.6
1	A	82	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	141	LYS	2.6
1	A	139	LEU	2.6
1	C	320	ILE	2.6
1	B	301	ALA	2.6
1	C	307	ALA	2.6
1	A	60	LYS	2.5
1	A	201	ARG	2.5
1	A	114	ALA	2.5
1	A	27	ALA	2.5
3	E	130	LYS	2.5
1	A	149	HIS	2.5
2	D	211	HIS	2.5
1	B	304	ASN	2.5
1	A	123	TYR	2.4
1	A	105	ARG	2.4
1	B	139	LEU	2.4
1	B	165	THR	2.4
1	C	237	VAL	2.4
2	D	278	VAL	2.4
1	C	260	ASN	2.4
1	C	243	THR	2.4
1	A	85	GLY	2.4
2	D	269	LEU	2.4
3	E	87	THR	2.4
1	C	330	GLN	2.4
1	A	167	LEU	2.4
1	B	96	ALA	2.3
1	C	98	ARG	2.3
1	A	90	LEU	2.3
2	D	273	PHE	2.3
1	C	357	LEU	2.3
1	C	368	PRO	2.3
2	D	10	ARG	2.3
3	E	115	THR	2.3
2	D	223	MET	2.3
3	E	1	MET	2.3
3	E	119	LEU	2.3
1	A	125	ILE	2.3
3	E	91	ASP	2.2
1	A	68	ILE	2.2
1	C	3	TYR	2.2
1	C	102	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	88	LEU	2.2
1	C	304	ASN	2.2
3	E	125	ALA	2.2
2	D	284	GLY	2.2
1	B	144	GLU	2.2
1	C	289	LEU	2.2
2	D	222	LEU	2.2
1	A	156	THR	2.2
1	B	121	LYS	2.2
1	C	24	VAL	2.2
1	C	37	ILE	2.2
1	B	89	ASP	2.2
1	B	2037	ILE	2.1
3	E	94	ARG	2.1
1	A	305	ASP	2.1
2	D	324	LEU	2.1
1	B	305	ASP	2.1
2	D	293	LEU	2.1
2	D	332	CYS	2.1
3	E	37	ASP	2.1
2	D	155	ALA	2.1
2	D	298	LEU	2.1
1	B	2019	VAL	2.1
1	B	159	PRO	2.1
1	A	205	LEU	2.1
1	A	109	ASP	2.1
2	D	268	PRO	2.1
1	A	80	ARG	2.1
1	A	87	PHE	2.1
1	A	119	ARG	2.1
3	E	141	PHE	2.1
1	B	143	LEU	2.1
2	D	24	LEU	2.1
1	B	163	PRO	2.0
1	B	88	VAL	2.0
1	B	214	LEU	2.0
3	E	248	LEU	2.0
1	A	7	ALA	2.0
1	B	171	LEU	2.0
1	A	106	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ZN	C	400	1/1	0.19	1.04	44,44,44,44	0
4	ZN	A	400	1/1	0.20	-0.07	130,130,130,130	0
4	ZN	B	400	1/1	0.16	-0.19	105,105,105,105	0
5	SO4	A	1500	5/5	0.14	-0.68	64,65,66,67	0
5	SO4	B	2500	5/5	0.15	-1.10	68,70,70,70	0
5	SO4	C	5500	5/5	0.17	-1.80	36,36,39,41	0
4	ZN	E	400	1/1	0.07	-1.84	156,156,156,156	0

6.5 Other polymers

There are no such residues in this entry.